=> file casreact
FILE 'CASREACT' ENTERED AT 15:37:05 ON 25 JAN 2005

FILE CONTENT:1840 - 23 Jan 2005 VOL 142 ISS 4

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* CASREACT now has more than 8 million reactions *
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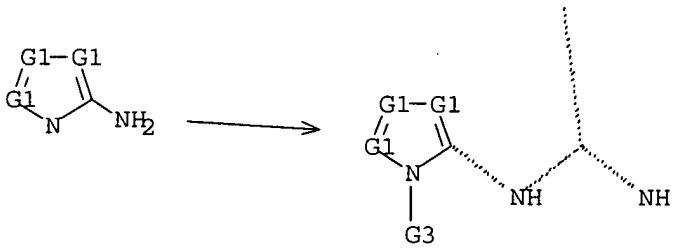
Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que
L1 STR



G1 C,N

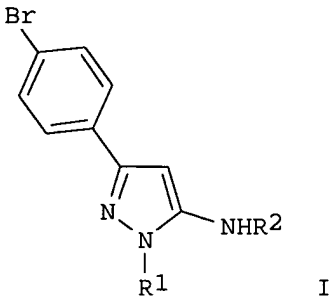
G2 O,S

G3 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.
L3 24 SEA FILE=CASREACT SSS FUL L1 (189 REACTIONS)

=> d l3 1-24 ibib abs fcrd

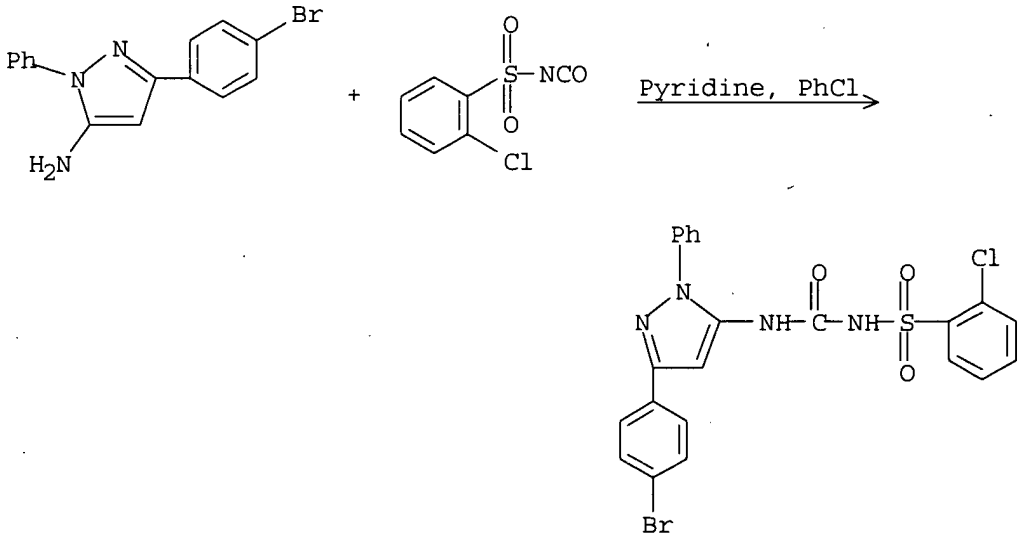
L3 ANSWER 1 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:395467 CASREACT
TITLE: 3-(p-Bromophenyl)-5-aminopyrazole and some derivatives
AUTHOR(S): Nam, N. L.; Grandberg, I. I.; Sorokin, V. I.
CORPORATE SOURCE: Kafedra Org. Khim., Timiryazevsk. S-Kh. Akad., Russia
SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi Akademii (2003), (4), 142-146
CODEN: ITSAA7; ISSN: 0021-342X
PUBLISHER: ANO "Izdatel'stvo MSKhA"
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I

AB 5-Aminopyrazoles I (R1 = H, Me, Ph; R2 = H) were readily prepared via cyanation of α,4-dibromoacetophenone with sodium cyanide followed by heterocyclization of 4-bromo-α-cyanoacetophenone with the corresponding hydrazines. Pyrazole I (R1 = Ph; R2 = H) was further functionalized by reactions with acyl and sulfonyl halides, anhydrides or isocyanates to give I (R1 = Ph; R2 = MeCO, PhCO, 4-MeC6H4SO2, 2-ClC6H4SO2NHCO).

RX(5) OF 19



73%

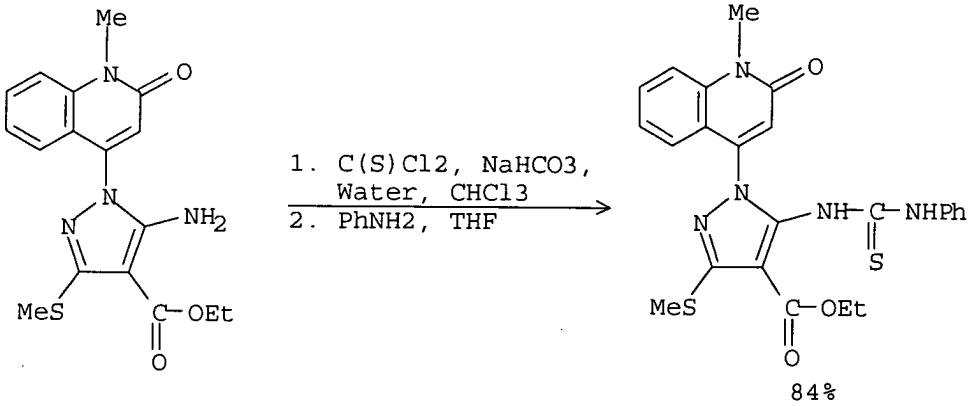
L3 ANSWER 2 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 140:59611 CASREACT
TITLE: Chemistry of Substituted Quinolinones. Part 8. Synthesis and Cyclization Reactions of Ethyl 5-Amino-1-(1-methyl-2-oxoquinolin-4-yl)-3-methylsulfanylpyrazole-4-carboxylate
AUTHOR(S): Abass, Mohamed
CORPORATE SOURCE: Ain Shams University, Cairo, Egypt
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (2003), 178(7), 1413-1432
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Taylor & Francis, Inc.

DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of the titled amino-ester I [R1 = Et; R2 = NH2(II)] is described and its hydrolysis and chloroacetylation led to the acid I (R1 = H; R2 = NH2) and acetamide I (R1 = Et; R2 = NHCOCH2Cl), which were cyclized to the pyrazolopyridones III (R = H) and III (R = Cl), resp. Condensation of II with 2,5-dimethoxytetrahydrofuran afforded the pyrrolylpyrazole I (R1 = Et; R2 = pyrrolo), which underwent cyclization by action of PPA to give pyrazolopyrrolizine IV. Treating II with thiophosgene gave the pyrazolyl isothiocyanate I (R1 = Et; R2 = NCS), which added aniline to yield the thiourea derivative I (R1 = Et; R2 = NHCSNHPh), and cyclized to give pyrazolopyrimidinethiones V (R = H, NH2, Ph). Condensation of II with formamide furnished pyrazolopyrimidine VI (R = H), while with tri-Et orthoformate produced the ethoxymethyleneaminopyrazole I (R1 = Et; R2 = N:CHOEt), which condensed with hydrazine to give the aminopyrazoloprimidine VI (R = NH2). Reaction of II with Lawesson's reagent resulted in the pyrazolothiazaphosphinine VII. Also the cyclization reaction of the compound II with malononitrile and its mixts. with carbon disulfide, Ph isothiocyanate, or benzaldehyde led to the formation of a variety of polyfunctional substituted pyrazolopyrimidines, pyrazolothiazine and pyrazolopyridine.

RX(41) OF 56 - 2 STEPS



84%

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 139:301299 CASREACT
TITLE: Structure-Activity Relationships of the p38α MAP Kinase Inhibitor 1-(5-tert-Butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-yl-ethoxy)naphthalen-1-yl]urea (BIRB 796)
AUTHOR(S): Regan, John; Capolino, Alison; Cirillo, Pier F.; Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Kroe, Rachel R.; Madwed, Jeffrey; Moriak, Monica; Nelson, Richard; Pargellis, Christopher A.; Swinamer,

Alan; Torcellini, Carol; Tsang, Michele; Moss, Neil
CORPORATE SOURCE: Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals Research and Development Center, Ridgefield, CT, 06877, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(22), 4676-4686
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We report on the structure-activity relationships (SAR) of 1-(5-tert-butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-yl-ethoxy)naphthalen-1-yl]urea (BIRB 796), an inhibitor of p38α MAP kinase which has advanced into human clin. trials for the treatment of autoimmune diseases. Thermal denaturation was used to establish mol. binding affinities for this class of p38α inhibitors. The tert-Bu group remains a critical binding element by occupying a lipophilic domain in the kinase which is exposed upon rearrangement of the activation loop. An aromatic ring attached to N-2 of the pyrazole nucleus provides important π-CH2 interactions with the kinase. The role of groups attached through an ethoxy group to the 4-position of the naphthalene and directed into the ATP-binding domain is elucidated. Pharmacophores with good hydrogen bonding potential, such as morpholine, pyridine, and imidazole, shift the melting temperature of p38α by 16-17° translating into Kd values of 50-100 pM. Finally, we describe several compds. that potently inhibit TNF-α production when dosed orally in mice.

RX(4) OF 120 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 139:85341 CASREACT
TITLE: Method for preparation of new N-substituted derivatives of 5-amino-1-phenylpyrazole, the derivatives, and their use as parasiticidal and/or insecticidal agents
INVENTOR(S): Bertrand, Guy; Romanenko, Vadim D.; Raynier, Bernard; Derrieu, Guy
PATENT ASSIGNEE(S): Virbac SA, Fr.
SOURCE: Fr. Demande, 87 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2834288	A1	20030704	FR 2001-17018	20011228

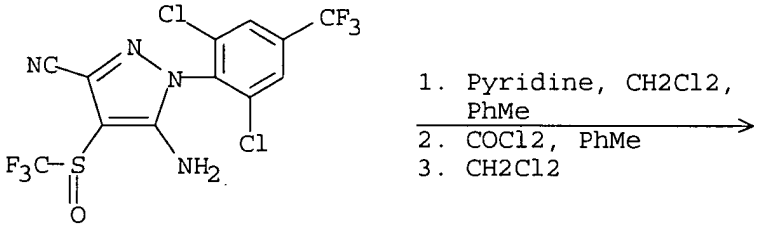
PRIORITY APPLN. INFO.: FR 2001-17018 20011228
OTHER SOURCE(S): MARPAT 139:85341
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

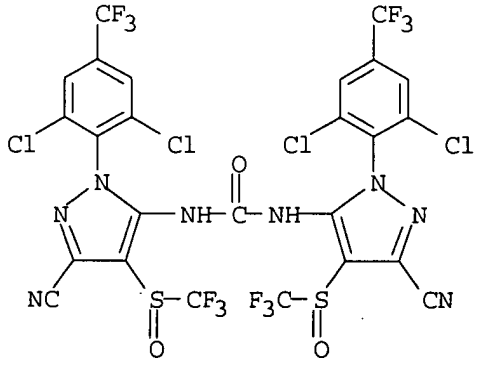
AB The invention provides new derivs. of 5-amino-1-phenylpyrazoles, specifically I [wherein: A, B = H, (a)cyclic alk(en/yn)yl (optionally

substituted by one or more halo, alkoxy, alkylthio, or alkoxycarbonyl), halo, cyano, thiocyano, nitro, sulfamido, (di)alkylamino, aminocarbonyl, aminothiocarbonyl, (di)alkylaminocarbonyl, (di)alkylaminothiocarbonyl, alkylcarbonylamino, alkylthiocarbonylamino, S(O)nR [n = 0, 1, or 2, and R = (a)cyclic, (un)saturated (halo)alkyl], Ph, phenylalkyl, or 4- to 7-membered heterocyclyl with 1-3 N/O/S/Si atom(s); R1, R2, R3, R4, and R5 = H, halo, (a)cyclic (un)saturated C1-6 (halo)alkyl, (halo)alkoxy, or (halo)alkylthio; Z = -N:C:O, -N:C:S, -N:S:O, -NHC(:X)R6, -NHC(:O)XR6, -NHC(:S)XR6, -NHC(:X)NR7R8; X = O or S; R6 = (un)substituted (a)cyclic alk(en/yn)yl, Ph, phenylalkyl, or heterocyclyl; R7, R8 = H, groups given for R6, dimeric unit of I; also Z = -N:C:N- forming a dimer of I; or Z = (un)substituted 1,2-thiazin-2-yl 1-oxide motif]. The invention also comprises processes for preparation of I from corresponding amines I [Z = NH2], typically via reaction of the amines with phosgene, thiophosgene, or thionyl chloride, and optionally reaction of the resultant I [Z = isocyanato, isothiocyanato, or N-sulfinylamino (i.e., -N:S:O)]. Compds. I can be administered to vertebrates, particularly domesticated animals, either orally, topically, or parenterally. In general, I can be used to control both arthropods and nematodes which are parasites of both animals and plants, by application to either the hosts or their environments. Over 30 specific compds. were claimed per se. Examples (23) include synthesis, and both agrochem. and pharmaceutical formulations. For instance, the amine precursor II [Z = NH2] reacted with phosgene in anhydrous PhMe in the presence of 2 equiv pyridine to give II [Z = isocyanato] in 95% yield. Reaction of this isocyanate with 3,5-bis(trifluoromethyl)aniline gave title compound III. Compds. I were against the stablefly Stomoxys calcitrans in a Petri dish experiment, at dosages of 0.1 to 30 μg/fly. An exemplary injectable contained 1% I, 30% Et oleate, and sesame oil qsp 100%, and was sterilized by membrane filtration.

RX(9) OF 11



(step 1)



92%

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 138:24709 CASREACT
TITLE: Preparation of pyrazole compds. and bis pyrazole-1H-pyrazole intermediates as antiinflammatory agents
INVENTOR(S): Kapadia, Suresh R.; Song, Jinhua J.; Yee, Nathan K.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: U.S., 37 pp., Cont.-in-part of U.S. 6,372,773.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6492529	B1	20021210	US 2002-67492	20020205
US 6319921	B1	20011120	US 2000-484638	20000118
US 6333325	B1	20011225	US 2001-871559	20010531
US 6329415	B1	20011211	US 2001-891579	20010626
US 2002065285	A1	20020530	US 2001-891820	20010626
US 6506748	B2	20030114		
US 6372773	B1	20020416	US 2001-920899	20010802
PRIORITY APPLN. INFO.:			US 2000-484638	20000118
			US 2001-920899	20010802
			US 1999-116400P	19990119
			US 2001-891579	20010626

OTHER SOURCE(S): MARPAT 138:24709
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Pyrazole compds., e.g. I, as well as bis pyrazole-1H-pyrazole intermediate compds. e.g. II, were prepared The compds. are useful in pharmaceutic compns. for treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases. All prepared compds. had IC50 < 10 mM for inhibition of TNFα in lipopolysaccharide stimulated THP cells.

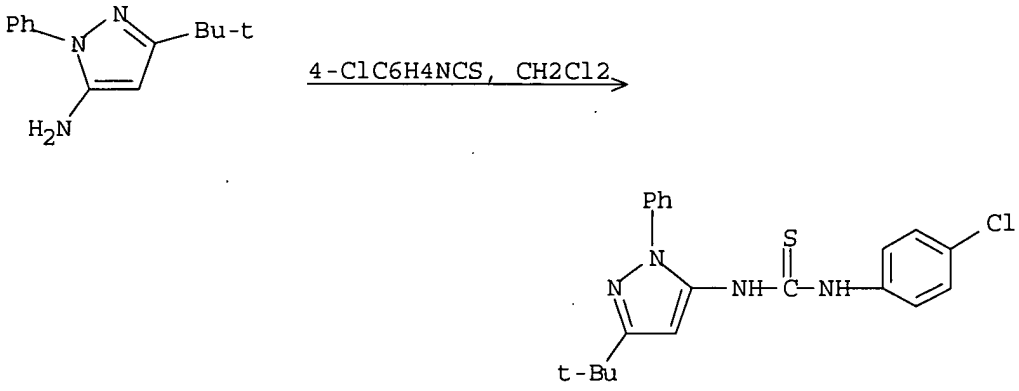
RX(1) OF 282 - REACTION DIAGRAM NOT AVAILABLE
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 137:119059 CASREACT
TITLE: Pyrazole Urea-Based Inhibitors of p38 MAP Kinase: From Lead Compound to Clinical Candidate
AUTHOR(S): Regan, John; Breitfelder, Steffen; Cirillo, Pier; Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Klaus, Bernhard; Madwed, Jeffrey; Moriak, Monica; Moss, Neil; Pargellis, Chris; Pav, Sue; Proto, Alfred; Swinamer, Alan; Tong, Liang; Torcellini, Carol
CORPORATE SOURCE: Research and Development Center, Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(14), 2994-3008
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We report on a series of N-pyrazole, N'-aryl ureas and their mode of binding to p38 mitogen activated protein kinase. Importantly, a key binding domain that is distinct from the ATP (ATP) binding site is exposed when the conserved activation loop, consisting in part of Asp168-Phe169-Gly170, adopts a conformation permitting lipophilic and hydrogen bonding interactions between this class of inhibitors and the protein. We describe the correlation of the structure-activity relationships and crystallog. structures of these inhibitors with p38. In addition, we incorporated another binding pharmacophore that forms a hydrogen bond at the ATP binding site. This modification affords significant improvements in binding, cellular, and in vivo potencies resulting in the selection of Compound 45 (BIRB 796) as a clin. candidate for the treatment of inflammatory diseases.

RX(7) OF 99

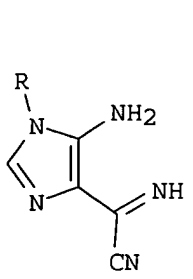


59%

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 135:211001 CASREACT
TITLE: A new and efficient approach to the synthesis of 6-amidino-2-oxopurines
AUTHOR(S): Booth, Brian L.; Cabral, Isabel M.; Dias, Alice M.; Freitas, A. Paula; Matos Beja, Ana M.; Proenca, M. Fernanda; Silva, Manuela Ramos
CORPORATE SOURCE: Department of Chemistry, UMIST, Manchester, M60 1QD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (10), 1241-1251
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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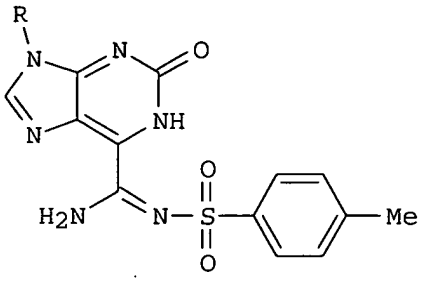

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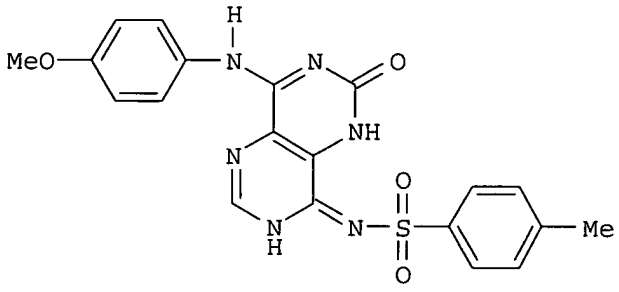
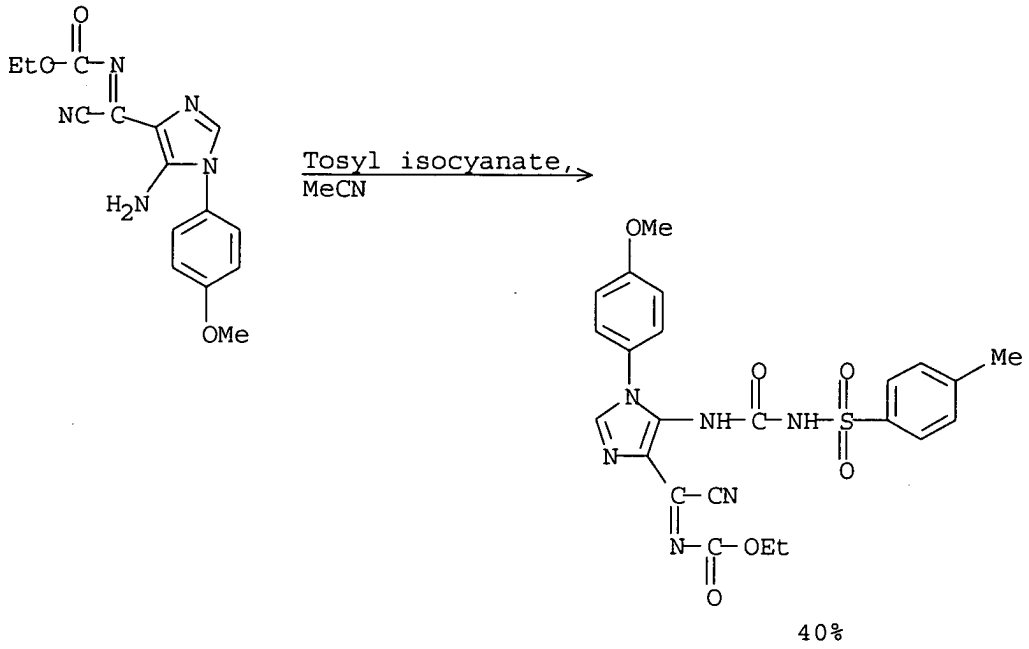


III

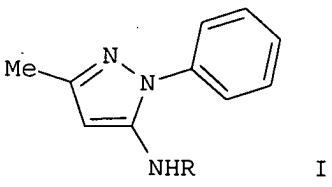
AB The reaction of 5-amino-4-cyanoformimidoylimidazoles I (R = HOCH2CH2, 4-MeOC6H4) with tosyl isocyanate proved to be a mild and efficient method for the synthesis of the corresponding 6-amidino-2-oxopurines II. These compds., which were isolated in almost quant. yield, rearrange in the presence of acetic acid-DMF to give a pyrimido[5,4-d]pyrimidin-2-one, e.g. III. The structure of compound III was confirmed by X-ray crystallog. The pathway for both reactions is discussed. Studies on the reactivity of tosyl isocyanate with imidazoles derived from I by selective acylation of the amino or imino nitrogen atoms, enabled clarification of the mechanism for purine formation.

RX(21) OF 41



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

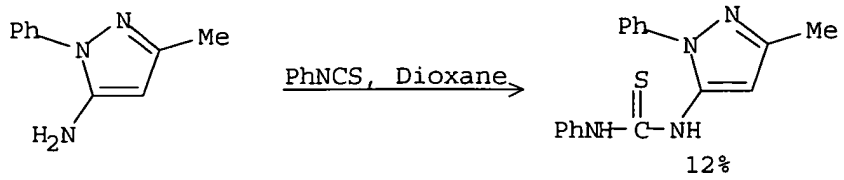
L3 ANSWER 8 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 134:340456 CASREACT
TITLE: Synthesis of N-acyl derivatives of 1-phenyl-3-methyl-5-aminopyrazole
AUTHOR(S): Nam, N. L.; Grandberg, I. I.; Sorokin, V. I.
CORPORATE SOURCE: Kafedra Org. Khim., Mosk. S-Kh. Akad. im. K. A. Timiryazeva, Moscow, Russia
SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi Akademii (2000), (1), 172-176
CODEN: ITSAA7; ISSN: 0021-342X
PUBLISHER: Izdatel'stvo MSKhA
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I

AB Aminopyrazole I (R = H), prepared from PhNHNH2·HCl and MeC:NHCH2CN, was N-acylated to give pyrazoles I (R = MeCO, PhCO, 4-ClC6H4CO, 4-BrC6H4CO, 4-MeC6H4SO2, PhNHCO, PhNHCS) in 47-78% yields.

RX(5) OF 15



12%

L3 ANSWER 9 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 134:237742 CASREACT

TITLE: Synthesis of sugar-modified derivatives of the unusual nucleoside oxanosine and its carbocyclic analogs as potential inhibitors of HIV

AUTHOR(S): Saito, Yoshio; Nakamura, Mariko; Ohno, Tsuneya; Chaicharoenpong, Chanya; Ichikawa, Eiko; Yamamura, Shosuke; Kato, Kuniki; Umezawa, Kazuo

CORPORATE SOURCE: Departments of Applied Chemistry and Chemistry, Keio University, Kohoku-ku, Yokohama, 223-0061, Japan

SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (3), 298-304
CODEN: JCSPCE; ISSN: 1472-7781

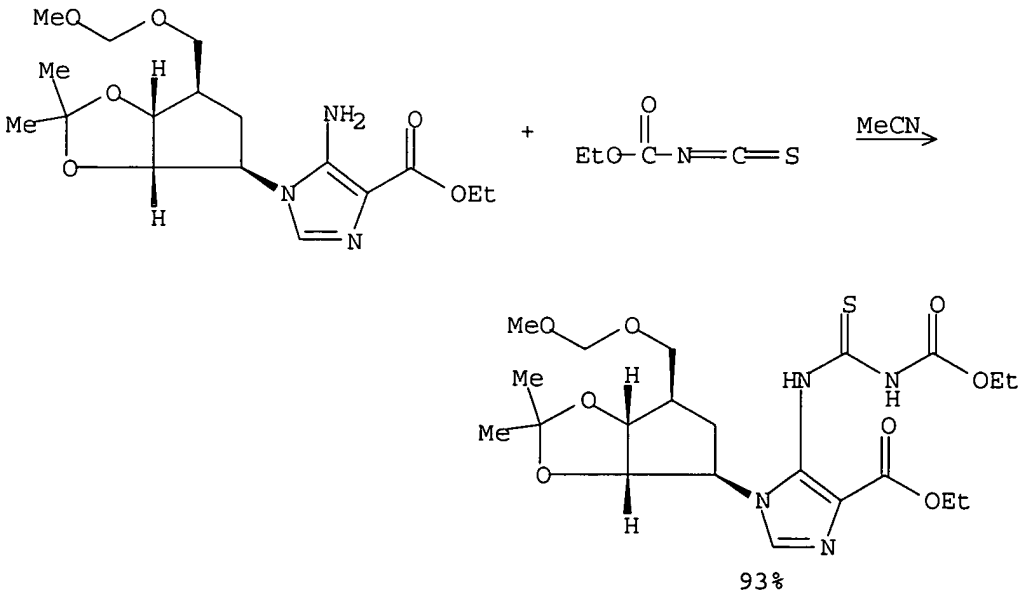
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of sugar-modified derivs. of oxanosine and its carbocyclic analogs were synthesized from natural oxanosine and (-)-2-azabicyclo[2.2.1]hept-5-en-3-one, resp. Among nucleosides tested for anti-HIV activities in vitro, oxanosine, its 5'-monophosphate, and 2'-deoxyoxanosine reduced the number of HIV particles in CEM cells to almost the same level as ddI.

RX(9) OF 52



93%

NOTE: stereoselective

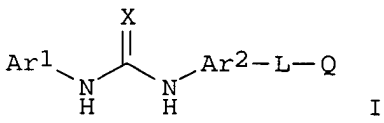
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 134:86264 CASREACT
TITLE: Novel process for synthesis of heteroaryl-substituted ureas
INVENTOR(S): Zhang, Lin-Hua; Zhu, Lei
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

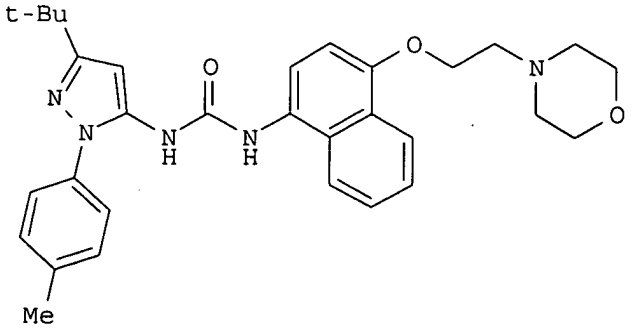
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001004115	A2	20010118	WO 2000-US17655	20000627
WO 2001004115	A3	20010927		
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2374737	AA	20010118	CA 2000-2374737	20000627
EP 1200411	A2	20020502	EP 2000-941745	20000627
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
JP 2003504366	T2	20030204	JP 2001-509725	20000627
US 6583282	B1	20030624	US 2000-611109	20000706
US 2003109703	A1	20030612	US 2002-300448	20021120
US 6753426	B2	20040622		
US 2003166930	A1	20030904	US 2003-361719	20030210
US 6774233	B2	20040810		
US 2003166931	A1	20030904	US 2003-361731	20030210
US 6835832	B2	20041228		
US 2003181718	A1	20030925	US 2003-361440	20030210

PRIORITY APPLN. INFO.: US 1999-143094P 19990709
WO 2000-US17655 20000627
US 2000-611109 20000706

OTHER SOURCE(S): MARPAT 134:86264
GI



I

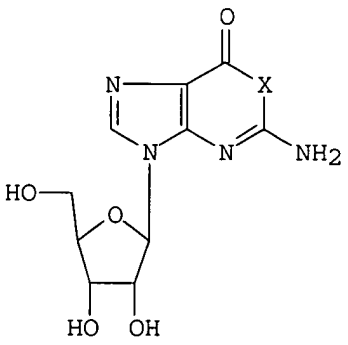


II

AB The title compds. [I; Ar1 = (un)substituted Ph, pyridinyl, pyrazolyl, etc.; Ar2 = (un)substituted Ph, naphthyl, quinolinyl, etc.; L = alkylene wherein one or more methylene groups are optionally replaced by O, N, or S, and substituted with 0-2 oxo groups and one or more alkyl, or L = cycloalkyl or cycloalkenyl optionally substituted with 1-2 oxo, 1-3 alkyl, alkoxy, alkylamino, etc., Q = (un)substituted Ph, naphthyl, pyridinyl, etc.; X = O, S], useful in pharmaceutic compns. for treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases (no data), were prepared E.g., a multi-step synthesis of the urea II was given.

RX(7) OF 9 - REACTION DIAGRAM NOT AVAILABLE

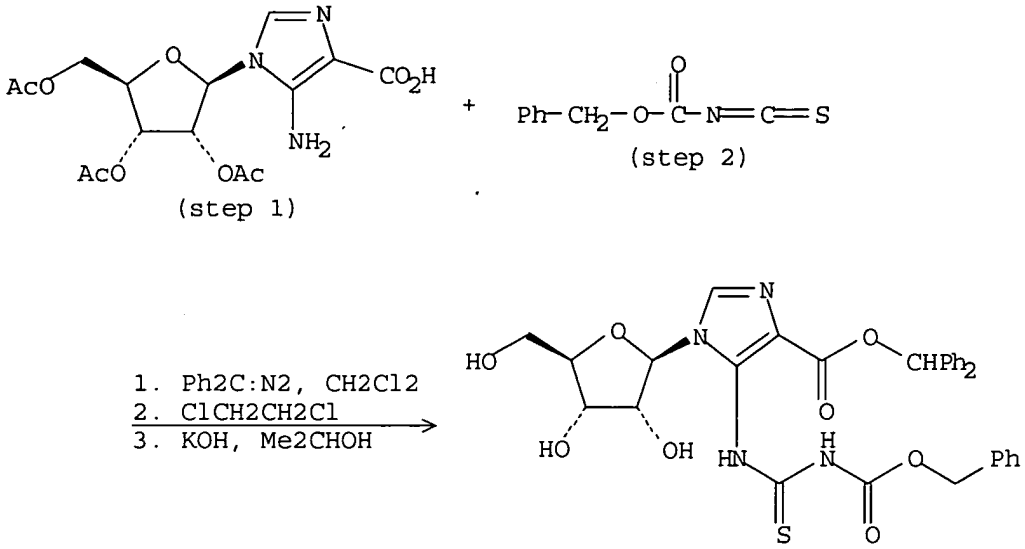
L3 ANSWER 11 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 120:324107 CASREACT
TITLE: A novel synthesis of oxanosine and 1-thiaguanosine
AUTHOR(S): Luk, Kin Chun; Moore, Douglas W.; Keith, Dennis D.
CORPORATE SOURCE: Roche Res. Cent., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Tetrahedron Letters (1994), 35(7), 1007-10
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A novel total synthesis of oxanosine I (X = O) has been developed. The key heterocycle forming reaction of this synthesis is the carbodiimide mediated dehydration and cyclization of an urea-acid derived from AICA-riboside. The same procedure was also applied to the synthesis of 1-thiaguanosine I (X = S). Antimicrobial activity of I against E. coli 257 was completely reversed by guanosine (no data).

RX(2) OF 6



L3 ANSWER 12 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 109:38166 CASREACT

TITLE: Enantioselective synthesis of new analogs of neplanocin A and their biological activity

AUTHOR(S): Arita, Masafumi; Okumoto, Takeki; Saito, Tadamasa; Hoshino, Yukio; Fukukawa, Kiyofumi; Shuto, Satoshi; Tsujino, Masatoshi; Sakakibara, Hideo; Ohno, Masaji

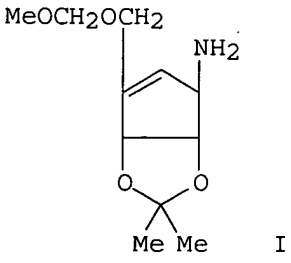
CORPORATE SOURCE: Res. Lab., Yoshitomi Pharm. Ind., Ltd., Iruma, 358, Japan

SOURCE: Carbohydrate Research (1987), 171, 233-58
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Various carbocyclic nucleosides analogs of neplanocin A; such as 5-aminoimidazole-4-carboxamide, riboside, uridine, 5-iodouridine, 4-thiouridine, cytidine, thymidine, 2'-deoxyguanosine, ribofuranosylthymine, a 2,2'-anhydroderiv., 2'-deoxycytidine, 2'-deoxythiouridine, and D-arabinofuranosylcytosine analogs were prepared from (1R,2S,3R)-2,3-isopropylidenedioxy-4-methoxymethyloxymethyl-4-cyclopenten-1-ylamine (I). The cytidine analog was found the most active in inhibiting mouse lymphoma L5178Y cells in vitro at a concentration as low as 0.8 μg/mL.

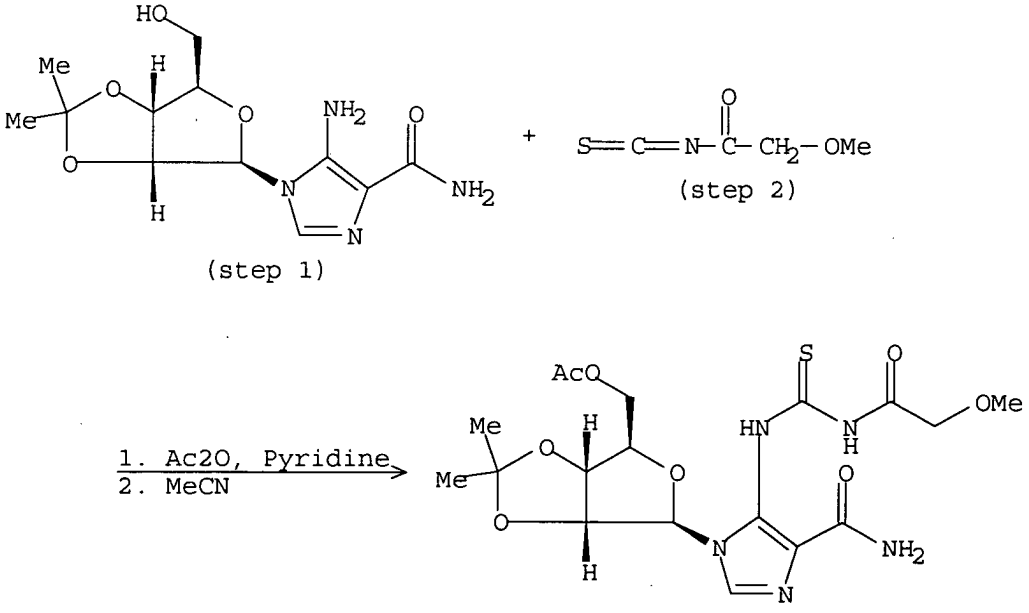
RX(3) OF 378 - REACTION DIAGRAM NOT AVAILABLE

L3 ANSWER 13 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 108:150875 CASREACT
TITLE: Conversion of the 2',3'-O-isopropylidene derivative of 5-amino-1-β-D-ribofuranosylimidazole-4-carboxamide (AICA riboside) into 2',3'-O-isopropylideneisoguanosine
AUTHOR(S): Reese, Colin B.; Sanghvi, Yogesh S.; Kuroda, Reiko
CORPORATE SOURCE: Dep. Chem., King's Coll., London, WC2R 2LS, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (7), 1527-31
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

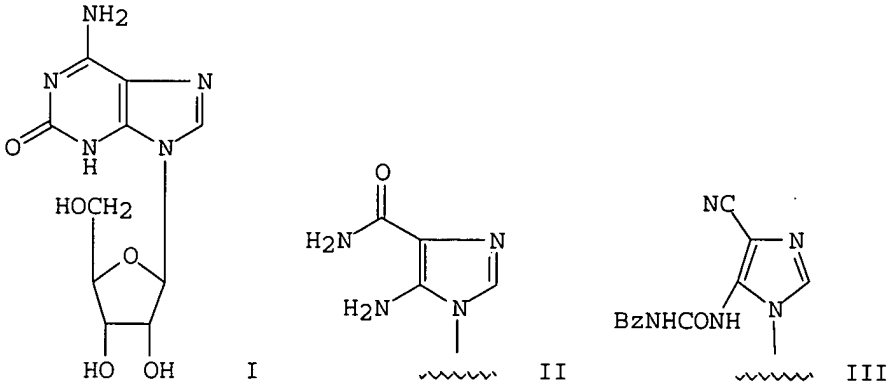
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Treatment of the putative methoxyacetylthioureido derivative I (R = COCH2OMe), which was prepared in 2 steps from 5-amino-1-(2',3'-O-isopropylidene-β-D-ribofuranosyl)imidazole-4-carboxamide, with Hg(ClO4)2 in the presence of pyridine in THF at room temperature and then with NH3-MeOH gives the ureido nitrile II (R = H) (III); treatment of I (R = H) with Hg2+ under the same conditions gives II (R = Ac). When III is allowed to react with (Me2N)2C:NH and H2O in THF at room temperature, 2',3'-O-isopropylideneisoguanosine (IV) is obtained in high yield; however, when III is heated, under reflux, with Et3N in dioxane-water, 5-amino-1-(2',3'-O-isopropylidene-β-D-ribofuranosyl)imidazole-4-carbonitrile is obtained in good yield.

RX(2) OF 22

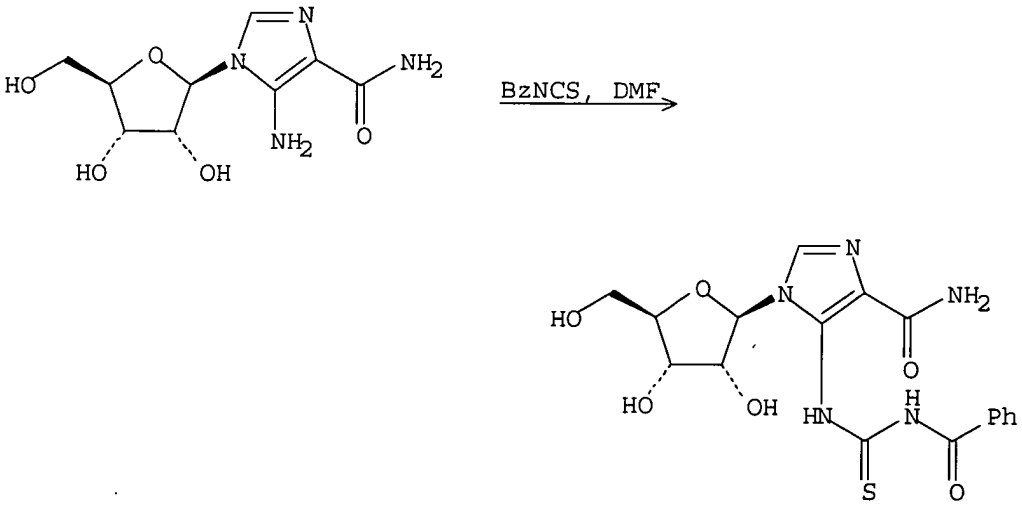


L3 ANSWER 14 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 108:38286 CASREACT
TITLE: Novel and efficient synthesis of isoguanosine
AUTHOR(S): Chern, Ji Wang; Lee, Horng Yuh; Huang, Min; Shish, Fang Jy
CORPORATE SOURCE: Med. Lab., Natl. Def. Med. Cent., Taipei, Taiwan
SOURCE: Tetrahedron Letters (1987), 28(19), 2151-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Isoguanosine (I) was prepared by a one-pot reaction involving a condensation of 5-amino-1-(β-D-ribofuranosyl)imidazole-4-carboxamide (II) with benzoyl isothiocyanate, treatment of the resulting thiourea derivative with N,N,'-dicyclohexylcarbodiimide furnished imidazolecarbonitrile III which was then annulated with ethanolic ammonia to afford I in a 68% yield from II.

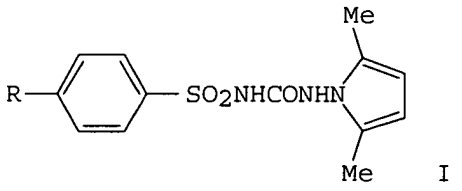
RX(4) OF 9



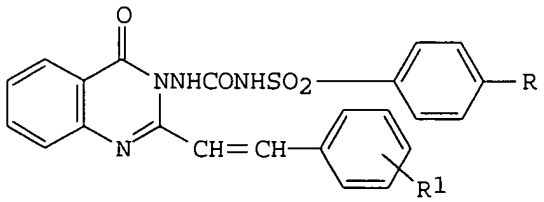
L3 ANSWER 15 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 107:58968 CASREACT

10/074,895

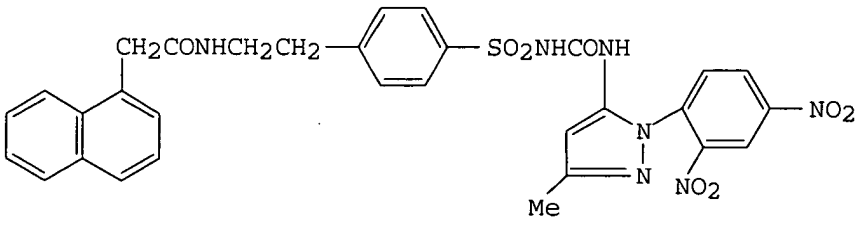
TITLE: Synthesis of some new substituted sulfonylureas as oral hypoglycemic agents
AUTHOR(S): Husain, M. I.; Srivastava, V. P.
CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 007, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(9), 934-8
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

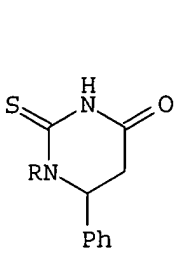


III

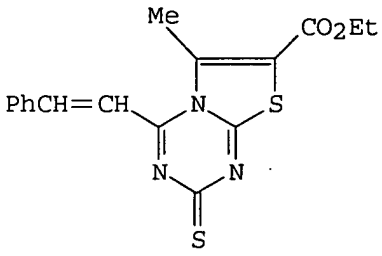
AB The title compds., e.g. I (R = H, Me, MeO, AcNH), II (R1 = 4-Me, 4-MeO, 4-Cl, 4-NO2) and III were prepared and their hypoglycemic activity evaluated. Some of these compds., when screened on albino rats at an oral dose of 250 mg/kg body weight, reduce the blood sugar to a significant extent.

RX(36) OF 107 - REACTION DIAGRAM NOT AVAILABLE

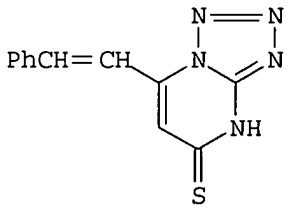
L3 ANSWER 16 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 106:119838 CASREACT
TITLE: A new convenient synthesis of 1,6-diaryl-2-thioxoperhydro-4-pyrimidinones: reaction of 3-phenyl-2-propenoyl isothiocyanate with aromatic and heteroaromatic amines
AUTHOR(S): Hafez, Ebtisam Abdel Aziz; Elmoghayar, Mohamed Rifaat Hamza; Ramiz, Mahmoud Mohamed Mahfouz
CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
SOURCE: Liebigs Annalen der Chemie (1987), (1), 65-7
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



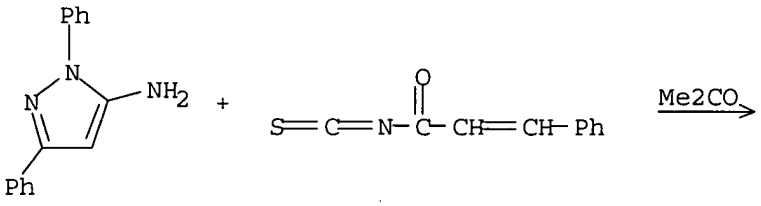
II

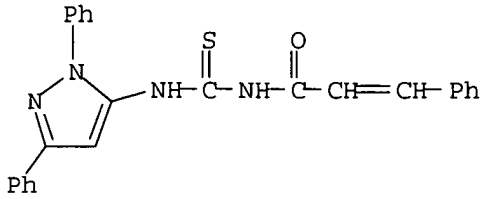


III

AB PhCH:CHCON:C:S was treated with RNH2 (R = Ph, p-O2NC6H4, p-MeOC6H4, Bu, PhCH2, 1,3-diphenyl-1H-pyrazol-5-yl, 3-phenyl-1H-pyrazol-5-yl, 5-ethoxycarbonyl-4-methyl-2-thiazolyl) to give PhCH:CHCONHCSNHR; which were cyclized by treatment with EtONa to give pyrimidinones I (R = Ph, p-O2NC6H4, 1,3-diphenyl-1H-pyrazol-5-yl) or thiazolotriazine II. PhCH:CHCON:C:S underwent cyclization with 1H-tetrazol-5-amine to give the tetrazolotriazine III.

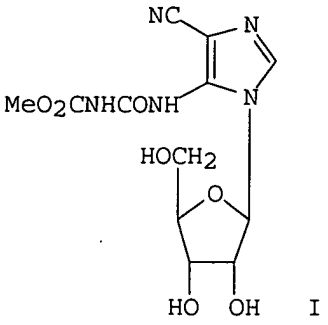
RX(6) OF 21





L3 ANSWER 17 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 105:60888 CASREACT
TITLE: An unexpected product from the cyclodesulfurization of 5-[1-(3-methoxycarbonyl)thioureido]-1-(β-D-ribofuranosyl)imidazole-4-carboxamide with dicyclohexylcarbodiimide
AUTHOR(S): Chern, Ji Wang; Groziak, Michael P.; Townsend, Leroy

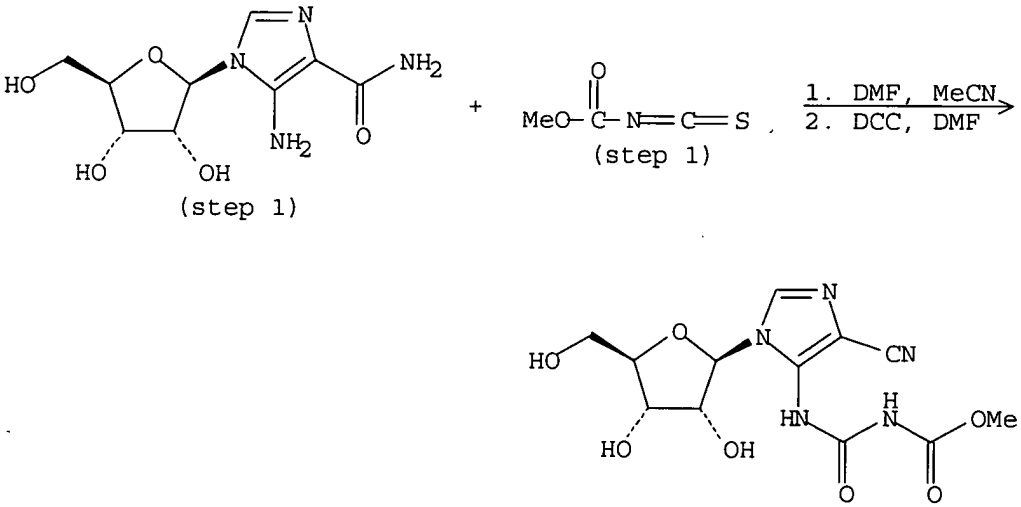
B.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109-1065, USA
SOURCE: Journal of Heterocyclic Chemistry (1986), 23(1), 153-4
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The treatment of 5-[1-(3-methoxycarbonyl)thioureido]-1-(β-D-ribofuranosyl)imidazole-4-carboxamide with N,N'-dicyclohexylcarbodiimide in DMF gave 4-cyano-5-[1-(3-methoxycarbonyl)-ureido]-1-(β-D-ribofuranosyl)imidazole (I).

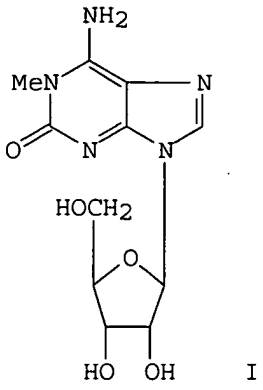
RX(1) OF 1



(step 1)

L3 ANSWER 18 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 105:60880 CASREACT
TITLE: A novel and efficient synthesis of the naturally occurring nucleoside doridosine
AUTHOR(S): Chern, Jiwang; Townsend, Leroy B.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109-1065, USA
SOURCE: Tetrahedron Letters (1985), 26(52), 6419-22

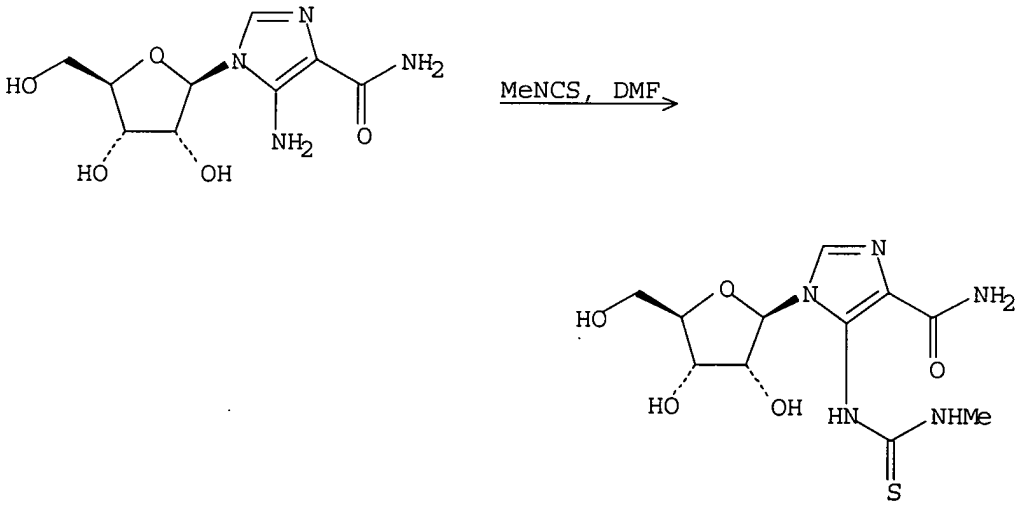
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB 1-Methylisoguanosine (doridosine, I) was prepared by a one-pot reaction involving a condensation of 5-amino-1-(β-D-ribofuranosyl)imidazole-4-carboxamide (II) with Me isothiocyanate, treatment of the resulting thiourea derivative with DCC furnished 5-(3-methyl-1-ureido)-1-(β-D-ribofuranosyl)imidazole-4-carbonitrile which was then annulated with ethanolic ammonia to furnish doridosine in a 68% yield from II.

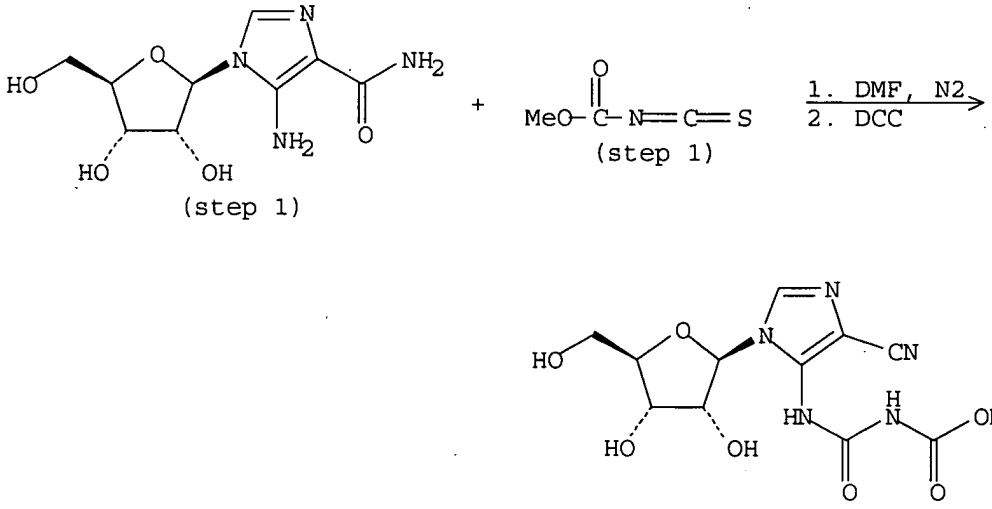
RX(1) OF 3



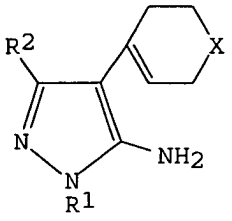
L3 ANSWER 19 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 104:149337 CASREACT
TITLE: Heterocyclic synthesis via a 1,3-dicyclohexylcarbodiimide-mediated cyclodesulfurative annulation reaction. New methodology for the preparation of guanosine and guanosine-type nucleoside analogs
AUTHOR(S): Groziak, Michael P.; Chern, Ji Wang; Townsend, Leroy

B.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI, 48109-1065, USA
SOURCE: Journal of Organic Chemistry (1986), 51(7), 1065-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Treatment of aminoribofuranosylimidazolecarboxamide (I, R = CONH2) with MeO2CNCS followed by cyclodesulfurization with DCC furnished [(methoxycarbonyl)ureido]ribofuranosylimidazolecarbonitrile (II, X = O). II (X = O, 18O) were also produced by hydrolysis of I (R = cyano) with H21802 and NH4OH followed by amidation and cyclodesulfurization, under similar reaction conditions. Me 5-amino-1-β-D-ribofuranosylimidazole-4-carboximidate affords 6-methoxy-2-[(methoxycarbonyl)amino]-9-β-D-ribofuranosylpurine, which gives guanosine upon deprotection with Me3SiI.

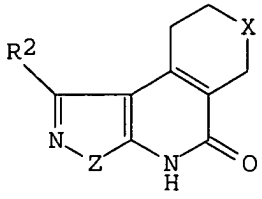
RX(1) OF 15



L3 ANSWER 20 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 103:37407 CASREACT
TITLE: Easy synthesis of new ring-fused pyridones from heteroaromatic β-vinylamines
AUTHOR(S): Winters, G.; Sala, A.; De Paoli, A.; Ferri, V.
CORPORATE SOURCE: Res. Lab., DOW-Lepetit, Milan, I-20158, Italy
SOURCE: Synthesis (1984), (12), 1052-4
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



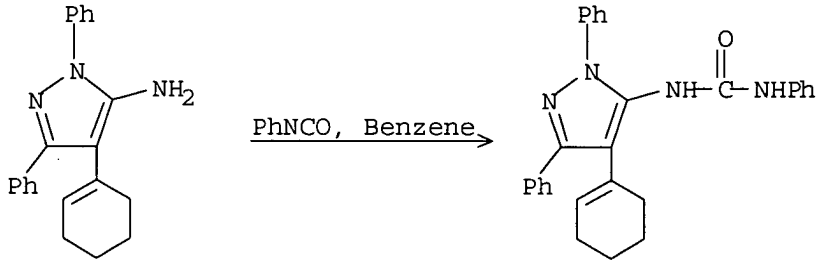
I



II

AB Cyclization of pyrazoles I (R1, R2 = Me, Ph; X = -, CH2, CH2CH2, NAc, NMe) with RNCO (R = Ph, Et) gave 75-98% cycloalkapyrazolopyridines II (Z = NR1). Similarly prepared were II (Z = O).

RX(2) OF 28



L3 ANSWER 21 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 101:55022 CASREACT

TITLE: Heterocyclic β-enamino esters. 31. Heterocyclic syntheses using dihalotriphenylphosphoranes. 6. New 6:7-, 6:8-, and 5:6:7-combinations of heterocondensed pyrimidines from iminophosphoranes of heterocyclic β-enamino esters. Stable heterocyclic ylides

AUTHOR(S): Wamhoff, Heinrich; Haffmanns, Guenter

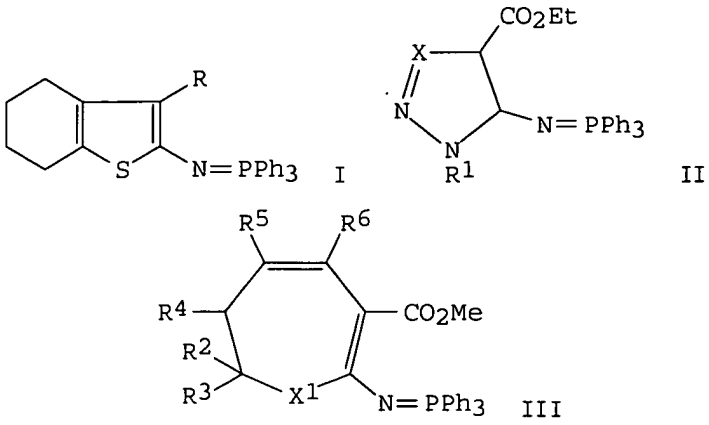
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1984), 117(2), 585-621
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

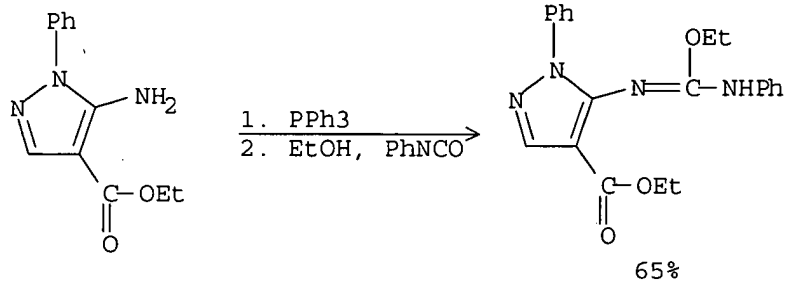
GI



I II III

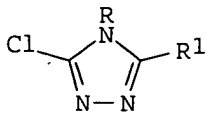
AB Tetrahydrobenzothiophenyliminophosphoranes I (R = CO2Et, cyano), heterocyclyliminophosphoranes II (X = CH, N; R1 = H, Ph, Me) and oxa- or thiacycloheptadienyliminophosphoranes III (X1 = O, S; R2, R3, R4 = H, Me; R5 = CO2Et, cyano; R6 = CO2Me, H) were prepared and their addition and cyclization reactions were studied. About 50 title pyrimidines were prepared

RX(74) OF 133 - 2 STEPS



65%

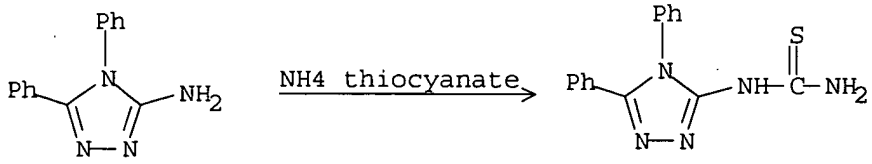
L3 ANSWER 22 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 87:201478 CASREACT
TITLE: Synthesis and reactivity of 4,5-disubstituted 3-chloro-1,2,4-triazoles and their methylsulfonyl analogs
AUTHOR(S): Nath, T. G. Surendra; Husain, Syeda; Srinivasan, V. R.
CORPORATE SOURCE: Dep. Chem., Osmania Univ., Hyderabad, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1977), 15B(4), 341-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



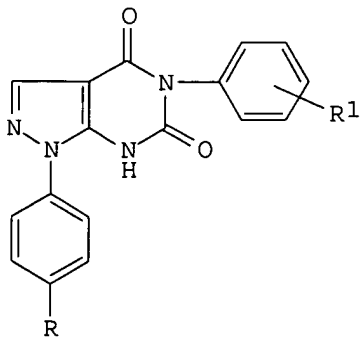
I

AB Several 4,5-disubstituted 3-chloro-1,2,4-triazoles I (R = Ph, 2-MeOC6H4, 2-, 3-, 4-MeC6H4; R1 = Ph, 2-MeOC6H4, 5-chloro-2-thienyl, 3-pyridyl, 4-MeC6H4) were prepared either by reaction of PCl5/POCl3 with the corresponding 3-hydroxytriazoles or by the oxidative chlorination of the corresponding 3-mercaptotriazoles. The Cl was replaced by H, mercapto, aryloxy, and amino groups to give variously substituted s-triazoles. The 3-methylsulfonyl analogs were prepared by the oxidation of the corresponding thioethers with KMnO4 in HOAc and their reactivity studied.

RX(3) OF 21



L3 ANSWER 23 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 86:29738 CASREACT
TITLE: Synthesis of some derivatives of pyrazolo[3,4-d]pyrimidine-4,6-diones
AUTHOR(S): Sarangan, S.; Somasekhara, S.
CORPORATE SOURCE: Med. Chem. Div., Sarabhai Res. Cent., Baroda, India
SOURCE: Journal of the Indian Chemical Society (1976), 53(4), 426-7
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

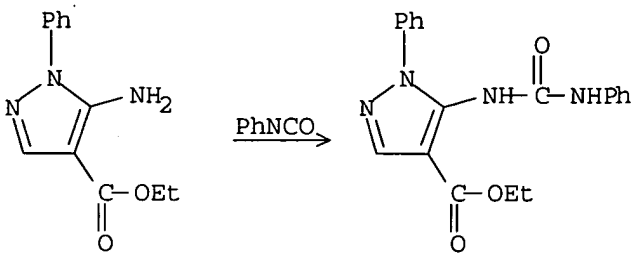


I

AB The pyrazolopyrimidinediones I (R = H, Me, Cl, MeO; R1 = H, o-Me, m-Me, p-Me, o-MeO, o-Cl, m-Cl) were prepared by cyclization of EtOCH:C(CN)CO2Et with p-RC6H4NHNH2 to give 1-phenyl-5-aminopyrazole-4-carboxylates, which were treated with R1C6H4NCO and the product ureido derivs. cyclized with

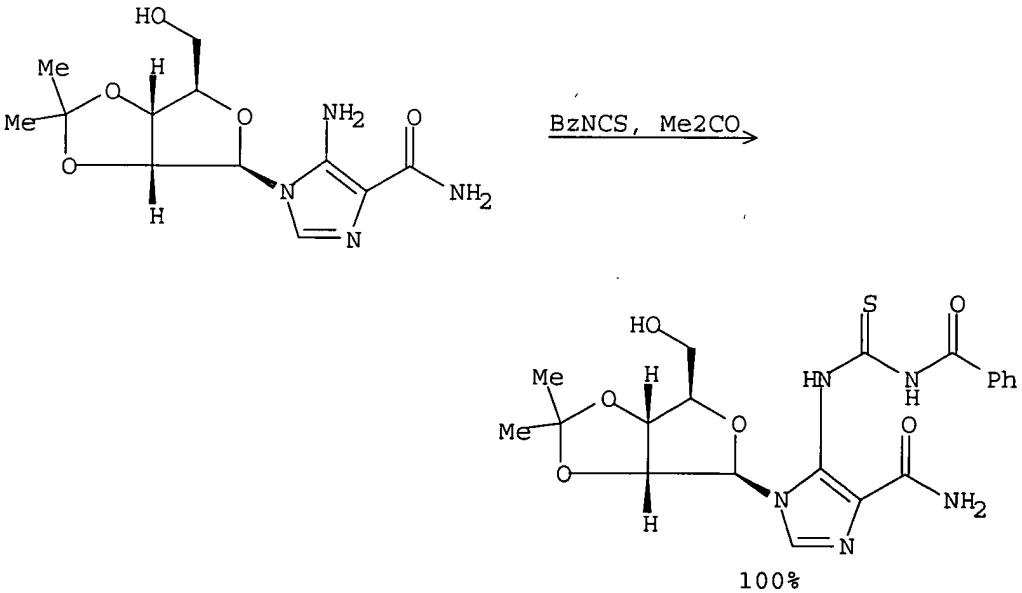
EtONa. At 200 mg/kg I (R = Me, R1 = m-Me) was antiinflammatory.

RX(2) OF 3



L3 ANSWER 24 OF 24 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 67:73818 CASREACT
TITLE: Synthesis of guanosine and its derivatives from 5-amino-1-(β-D-ribofuranosyl)-4-imidazolecarboxamide. I. Ring closure with benzoyl isothiocyanate
AUTHOR(S): Yamazaki, Akihiro; Kumashiro, Izumi; Takenishi, Tadao
CORPORATE SOURCE: Ajinomoto Co., Inc., Kawasaki, Japan
SOURCE: Journal of Organic Chemistry (1967), 32(6), 1825-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Guanine (I) was synthesized by condensation of 5-amino-4-imidazolecarboxamide with BzNCS followed by methylation and ring closure. This method has also been applied to the synthesis of 2',3'-O-isopropylideneguanosine from 5-amino-1-(2,3-O-isopropylidene-β-D-ribofuranosyl)-4-imidazolecarboxamide.

RX(2) OF 2



100%

NOTE: Classification: N-Acylation; Addition; Chemoselective; #
Conditions: acetone Rf 1h